Energy and Momentum Conserving Algorithms
in Continuum Mechanics

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INTRODUCTION

MAIN CONCERN

Time integration of the general system

\[ \dot{z} = J(z) \nabla H(z) - D(z) \nabla H(z) \]

\[ z \in \mathbb{R}^m, \quad H : \mathbb{R}^m \to \mathbb{R}, \]

\[ J = -J^T \in \mathbb{R}^{m \times m}, \quad D = D^T \geq 0 \in \mathbb{R}^{m \times m} \]

- includes general Hamiltonian systems
- analogous infinite-dimensional case
KEY FEATURES

Energy decay/conservation

\[ \dot{H} = \nabla H \cdot \dot{z} = \nabla H \cdot [J \nabla H - D \nabla H] \]

\[ \dot{H} = -\nabla H \cdot D \nabla H \leq 0 \quad \text{and} \quad \dot{H} = 0 \quad \text{when} \quad D \equiv O \]

Momentum conservation (linear/angular momentum)

Suppose

- \( H = \hat{H} \circ \zeta \)
- \( \zeta : R^m \rightarrow R^k \) invariants under a symmetry group, e.g.
  \[ \zeta(z) = (|q|^2, q \cdot p, |p|^2), \quad z = (q, p) \in R^6 \]
  "rotational invariants"

- \( \exists F(z) \) such that \( J \nabla F \in \ker[\nabla \zeta] \)

Then

\[ \dot{F} = 0 \quad \text{when} \quad D \equiv O \]
OBJECTIVE & MOTIVATION

OBJECTIVE

To develop time integration schemes with:

- mild or no restrictions on time step (stable implicit schemes)
- energy/momentum conservation when no damping present
- physical energy decay when damping present

MOTIVATION

- classic schemes generally fail on all three points
**EXAMPLE:** \( \dot{H} = 0 \)

Nonlinear Shells (Simo & Tarnow 1992)

**Energy vs Time:** Mid-Point Rule & Trapezoidal Rule

![Energy vs Time Graphs](image-url)
I. Introduction and motivation

II. Why does the Mid-Point Rule fail?
   - Kepler model problem
   - Elastodynamics model problem
     - Illustration of difficulties
     - Remedies

III. Abstract framework for conserving schemes
   - Discrete gradients
   - General scheme

IV. Closing remarks
KEPLER MODEL PROBLEM

\[ \dot{q} = m^{-1}p \]
\[ \dot{p} = -\frac{V'(|q|)}{|q|}q \]

\[ z = (q, p), \quad H(z) = \frac{1}{2}m^{-1}|p|^2 + V(|q|), \quad J = \begin{pmatrix} O & I \\ -I & O \end{pmatrix} \]

FEATURES

- \( H(z) \) invariant under rotation group
- \( H(z), \quad j(z) = q \times p \) are integrals
- \( q, p \in \mathbb{R}^3 \) evolve in plane normal to \( \mu = j(z_0) \)
- the radial variables \( \lambda = |q| \) and \( \pi = p \cdot q/|q| \) satisfy

\[ \dot{\lambda} = m^{-1}\pi \]
\[ \dot{\pi} = -V'_\mu(\lambda) \]

"reduced equations"

where

\[ V_\mu(\lambda) = V(\lambda) + \frac{1}{2}|\mu|^2/m\lambda^2 \]

"Smale’s amended potential"
**Relative Equilibria**

steady, circular orbit

\[
\dot{q} = m^{-1} p \\
\dot{p} = -\frac{V'(|q|)}{|q|} q
\]

fixed point

\[
\dot{\lambda} = m^{-1} \pi \\
\dot{\pi} = -V''(\lambda) \\
V''(\lambda^*) = 0
\]

**Stability**

stable relative equilibria = stable fixed point

= local min of \( V_\mu(\lambda) \)
Analysis of the Mid-Point Rule

**Mid-Point Rule**

\[
\begin{align*}
\frac{q_{n+1} - q_n}{\Delta t} &= m^{-1}p_{n+\frac{1}{2}} \\
\frac{p_{n+1} - p_n}{\Delta t} &= -\frac{V'(|q_{n+\frac{1}{2}}|)}{|q_{n+\frac{1}{2}}|}q_{n+\frac{1}{2}}
\end{align*}
\]

(1)

where \(q_{n+\frac{1}{2}} = \frac{1}{2}(q_{n+1} + q_n)\).

- preserves \(j(z_n) = q_n \times p_n\)
- does not preserve \(H(z_n) = \frac{1}{2}m^{-1}|p_n|^2 + V(|q_n|)\).

**Reduced Equations**

Introduce reduced variables as before

\[\lambda_n = |q_n|, \quad \pi_n = p_n \cdot q_n/|q_n|.\]

Then (1) implies the implicit reduced equation

\[G_{MP}(\lambda_{n+1}, \pi_{n+1}; \lambda_n, \pi_n) = 0.\]

(2)

- look for fixed points \((\hat{\lambda}^*, 0) \Leftrightarrow \) relative equilibria
- study stability
RESUL TS

Existence of Relative Equilibria:

Fixed points $\hat{\lambda}^*$ are stationary points of a perturbed potential:

$$\hat{V}_\mu(\lambda, \Delta t) \approx V_\mu(\lambda)$$

Stability of Relative Equilibria:

Fixed points $\hat{\lambda}^*$ are only conditionally stable in general:

- linearly stable when $\Delta t < \Delta t_{critical}$
- unstable when $\Delta t > \Delta t_{critical}$

Two questions:

- What’s causing the instability?
- Is there a cure?
**SOURCE OF INSTABILITY**

coupling between internal forces and rotations

Exact Problem:

\[
\frac{V'(|q|)}{|q|} \text{ rotationally invariant when } q = \Lambda(t)q_0
\]

Mid-point discretization:

\[
\frac{V'(|q_{n+\frac{1}{2}}|)}{|q_{n+\frac{1}{2}}|} \text{ not rotationally invariant when } q_{n+1} = \Lambda q_n
\]

\[n+1\]
\[n+1/2\]
\[n\]

**A REMEDY**

replace

\[
V'(|q_{n+\frac{1}{2}}|) \quad \frac{1}{|q_{n+\frac{1}{2}}|}
\]

by

\[
\frac{V(|q_{n+1}|) - V(|q_n|)}{|q_{n+1}| - |q_n|} \quad \frac{1}{\frac{1}{2}(|q_{n+1}| + |q_n|)}
\]
A Conserving Scheme

**Conserving Scheme**

\[
\begin{align*}
\frac{q_{n+1} - q_n}{\Delta t} &= m^{-1} p_{n+\frac{1}{2}} \\
\frac{p_{n+1} - p_n}{\Delta t} &= -\frac{V(|q_{n+1}|) - V(|q_n|)}{|q_{n+1}| - |q_n|} \left( \frac{q_{n+\frac{1}{2}}}{\frac{1}{2}(|q_{n+1}| + |q_n|)} \right)
\end{align*}
\]  

\[ (3) \]

- preserves \( j(z_n) = q_n \times p_n \)
- preserves \( H(z_n) = \frac{1}{2} m^{-1}|p_n|^2 + V(|q_n|) \).

**Reduced Equations**

Introduce reduced variables as before

\[ \lambda_n = |q_n|, \quad \pi_n = p_n \cdot \frac{q_n}{|q_n|}. \]

Then (3) implies the implicit reduced equation

\[ G_{EM}(\lambda_{n+1}, \pi_{n+1}; \lambda_n, \pi_n) = 0 \]  

\[ (4) \]

- look for fixed points \( (\hat{\lambda}^*, 0) \) \Leftrightarrow \relative equilibria
- study stability
RESULTS

Existence of Relative Equilibria:

Fixed points \( \hat{\lambda}^* \) are exact, i.e. stationary points of \( V_{\mu}(\lambda) \).

Stability of Relative Equilibria:

i. The reduced equations preserve the integral

\[
H_{\mu}(\lambda, \pi) = \frac{1}{2} m^{-1} \pi^2 + V_{\mu}(\lambda) \quad \text{“reduced Hamiltonian”}
\]

ii. \( V_{\mu} \) local min at \( \hat{\lambda}^* \) \( \Rightarrow \) \( H_{\mu} \) local min at \( (\hat{\lambda}^*, 0) \)

\( \Rightarrow \) \( H_{\mu} \) is a Lyapunov function

\( \Rightarrow \) nonlinear stability.

Three remarks on conserving scheme:

- 2nd order accurate, like Mid-Point rule
- “conserving” modification cures coupling/stability problem
- similar problem/cure in more complex systems
ELASTODYNAMICS MODEL PROBLEM

\[ \varphi(\ast, t) \]

\[ \Omega \]

\[ \mathbb{R}^3 \]

\[ \pi(X,t) \]

\[ \phi(X,t) \]

Notation

Deformation \( \varphi : \tilde{\Omega} \times [0, T] \rightarrow \mathbb{R}^3 \)

(Linear) Momentum Density \( \pi : \tilde{\Omega} \times [0, T] \rightarrow \mathbb{R}^3 \)

Deformation Gradient \( F(\varphi) = \nabla \varphi \)

Cauchy Strain \( C(\varphi) = F(\varphi)^T F(\varphi) \)

Strain Energy Function \( W(C) \)

Second Piola-Kirchhoff Stress \( \Sigma(\varphi) \)

\[ \Sigma(\varphi) = 2 \, DW(C(\varphi)) \]
Find $\varphi, \pi : \bar{\Omega} \times [0, T] \to \mathbb{R}^3$ such that

\[
\begin{align*}
\dot{\varphi} &= \rho^{-1} \pi & \text{in} & \quad \Omega \times (0, T) \\
\dot{\pi} &= \nabla \cdot [F(\varphi) \Sigma(\varphi)] + b & \text{in} & \quad \Omega \times (0, T) \\
\varphi &= g & \text{in} & \quad \Gamma_{\varphi} \times (0, T) \\
F(\varphi) \Sigma(\varphi) N &= h & \text{in} & \quad \Gamma_{\Sigma} \times (0, T)
\end{align*}
\]

plus initial conditions
Key Features

- Infinite-dimensional version of general system with
  \[ z = (\varphi, \pi), \quad J = \begin{pmatrix} O & I \\ -I & O \end{pmatrix} \]
  \[ H(z) = \int_\Omega \left[ \frac{1}{2} \rho^{-1} |\pi|^2 + W(C(\varphi)) - \varphi \cdot b \right] d\Omega \]
  \[ -\int_{\Gamma_\Sigma} \varphi \cdot h \, d\Gamma \]

- Typical integrals

  Energy \quad H(z)

  Linear Momentum \quad l(z) = \int_\Omega \pi \, d\Omega

  Angular Momentum \quad j(z) = \int_\Omega \varphi \times \pi \, d\Omega

Note: For the Neumann problem with no external loads

  i.e. \quad \Gamma_\Sigma = \partial \Omega, \quad h = 0 \quad and \quad b = 0

all of the above quantities are integrals.
Mid-Point Rule Time Discretization

Given \( \varphi_n, \pi_n \) find \( \varphi_{n+1}, \pi_{n+1} \) such that

\[
\frac{\varphi_{n+1} - \varphi_n}{\Delta t} = \rho^{-1} \pi_{n+\frac{1}{2}} \quad \text{in} \quad \Omega \\
\frac{\pi_{n+1} - \pi_n}{\Delta t} = \nabla \cdot [F(\varphi_{n+\frac{1}{2}}) \Sigma(\varphi_{n+\frac{1}{2}})] + b \quad \text{in} \quad \Omega \\
\varphi_{n+\frac{1}{2}} = g \quad \text{on} \quad \Gamma_{\varphi} \\
F(\varphi_{n+\frac{1}{2}}) \Sigma(\varphi_{n+\frac{1}{2}}) N = h \quad \text{on} \quad \Gamma_{\Sigma}
\]

where \((\cdot)_{n+\frac{1}{2}} = \frac{1}{2}[(\cdot)_n + (\cdot)_{n+1}]\) and \(\Delta t > 0\) is the time step.

- time discretization reduces the IBVP to a sequence of BVPs for \( \varphi_{n+1}, \pi_{n+1} \) \((n = 0, 1, 2, \ldots)\)
- each BVP may be solved using a finite-element method
- scheme preserves \( l \) and \( j \), but in general not \( H \)
**Numerical Example**

**Pinched Rubber Quarter-Cylinder**

- Stored Energy Function: three-term Ogden model

\[
W(C) = \sum_{A=1}^{3} \sum_{m=1}^{3} \frac{\mu_m}{\alpha_m} [\lambda_A^{\alpha_m}(C) - 1] - \mu_m \ln[\lambda_A(C)]
\]

where \(\lambda_A^2(C) > 0\) \((A = 1, 2, 3)\) are the eigenvalues of \(C \in S_{PD}^3\).

- Spatial Discretization: FEM with 512 trilinear bricks (2295 dof).
Implicit Mid-Point Rule with Time Step $\Delta t = 0.0005s$

$t = 0.0035s$

$t = 0.0050s$

$t = 0.0070s$

$t = 0.0090s$
Implicit Mid-Point Rule with Time Step $\Delta t = 0.0005s$

Angular Momentum and Energy Histories

\[
\begin{align*}
J_1 &: -5e-06, -4e-06, -3e-06, -2e-06, -1e-06, 0 \\
J_2 &: -0.002, -0.003, -0.004, -0.005, 0 \\
J_3 &: -4e-05, -3e-05, -2e-05, -1e-05, -8e-05, 0 \\
H &: 1.1, 1.2, 1.3, 1.4, 1.5, 1.6, 1.7, 1.8, 1.9, 2.0
\end{align*}
\]
Implicit Mid-Point Rule with Time Step $\Delta t = 0.0002s$

Angular Momentum and Energy Histories

\[ J_1 \]
\[ J_2 \]
\[ J_3 \]
\[ H \]
Character of Solution During Energy Growth

$t = 0.0500s$

$t = 0.0505s$

$t = 0.0510s$

$t = 0.0515s$
A Familiar Difficulty

Exact Problem:

\[ \Sigma(\varphi) = 2 \, DW(C(\varphi)) \]

invariant when \( \varphi = \Lambda(t)\varphi_0 \)

Mid-point discretization:

\[ \Sigma(\varphi_{n+\frac{1}{2}}) = 2 \, DW(C(\varphi_{n+\frac{1}{2}})) \]

not invariant when \( \varphi_{n+1} = \Lambda\varphi_n \)

A Remedy

replace \( DW(C(\varphi_{n+\frac{1}{2}})) \)

by \( dW(C_n, C_{n+1}) \approx DW(C(\varphi_{n+\frac{1}{2}})) \) where \( C_n = C(\varphi_n) \)
A Conserving Scheme

\[
\frac{\varphi_{n+1} - \varphi_n}{\Delta t} = \rho^{-1} \pi_{n+\frac{1}{2}} \quad \text{in } \Omega \\
\frac{\pi_{n+1} - \pi_n}{\Delta t} = \nabla \cdot [F(\varphi_{n+\frac{1}{2}})\tilde{\Sigma}] + b \quad \text{in } \Omega \\
\varphi_{n+\frac{1}{2}} = g \quad \text{on } \Gamma_{\varphi} \\
F(\varphi_{n+\frac{1}{2}})\tilde{\Sigma}N = h \quad \text{on } \Gamma_{\Sigma}
\]

where

\[
\tilde{\Sigma} \overset{\Delta}{=} 2 \, dW(C_n, C_{n+1})
\]

\[
dW(C_n, C_{n+1}) \overset{\Delta}{=} DW(C_{n+\frac{1}{2}}) + \left[ \frac{W(C_{n+1}) - W(C_n) - DW(C_{n+\frac{1}{2}}) : M}{||M||^2} \right] M
\]

and \(M \overset{\Delta}{=} C_{n+1} - C_n\).

- \(dW(C_n, C_{n+1})\) is a “discrete gradient”
- conserves \(l, j\) and \(H\)
Conserving Scheme with Time Step $\Delta t = 0.0005s$

Angular Momentum and Energy Histories

![Graphs showing angular momentum and energy histories.](image-url)
Comparison of Mid-Point and Conserving Schemes

**Mid-Point**

- $t=0.0500s$
  - **STRESS 3**
    - Min = $-2.61 \times 10^6$
    - Max = $1.37 \times 10^6$
    - Color Scale:
      - -2.04E+06
      - -1.48E+06
      - -9.08E+05
      - -3.40E+05
      - 2.29E+05
      - 7.97E+05

- $t=0.0495s$
  - **STRESS 3**
    - Min = $-1.58 \times 10^6$
    - Max = $1.08 \times 10^6$
    - Color Scale:
      - -1.20E+06
      - -8.17E+05
      - -4.38E+05
      - -5.89E+04
      - 3.20E+05
      - 6.99E+05

- $t=0.0505s$
  - **STRESS 3**
    - Min = $-1.34 \times 10^6$
    - Max = $1.34 \times 10^6$
    - Color Scale:
      - -9.54E+05
      - -5.72E+05
      - -1.90E+05
      - 1.92E+05
      - 5.74E+05
      - 9.56E+05

- $t=0.0500s$
  - **STRESS 3**
    - Min = $-3.11 \times 10^5$
    - Max = $6.57 \times 10^5$
    - Color Scale:
      - -1.73E+05
      - -3.42E+04
      - 1.04E+05
      - 2.42E+05
      - 3.81E+05
      - 5.19E+05

- $t=0.0510s$
  - **STRESS 3**
    - Min = $-6.18 \times 10^5$
    - Max = $1.22 \times 10^6$
    - Color Scale:
      - -3.56E+05
      - -9.33E+04
      - 1.69E+05
      - 4.32E+05
      - 6.94E+05
      - 9.56E+05

- $t=0.0515s$
  - **STRESS 3**
    - Min = $-2.65 \times 10^6$
    - Max = $9.58 \times 10^5$
    - Color Scale:
      - -2.13E+06
      - -1.62E+06
      - -1.10E+06
      - -5.87E+05
      - 7.21E+05
      - 4.43E+05

**Conserving**

- $t=0.0495s$
  - **STRESS 3**
    - Min = $-1.58 \times 10^6$
    - Max = $1.08 \times 10^6$
    - Color Scale:
      - -1.20E+06
      - -8.17E+05
      - -4.38E+05
      - -5.89E+04
      - 3.20E+05
      - 6.99E+05

- $t=0.0500s$
  - **STRESS 3**
    - Min = $-3.11 \times 10^5$
    - Max = $6.57 \times 10^5$
    - Color Scale:
      - -1.73E+05
      - -3.42E+04
      - 1.04E+05
      - 2.42E+05
      - 3.81E+05
      - 5.19E+05

- $t=0.0505s$
  - **STRESS 3**
    - Min = $-8.81 \times 10^5$
    - Max = $7.01 \times 10^5$
    - Color Scale:
      - -6.55E+05
      - -4.29E+05
      - -2.03E+05
      - 2.28E+04
      - 2.49E+05
      - 4.75E+05

- $t=0.0510s$
  - **STRESS 3**
    - Min = $-8.81 \times 10^5$
    - Max = $7.01 \times 10^5$
    - Color Scale:
      - -6.55E+05
      - -4.29E+05
      - -2.03E+05
      - 2.28E+04
      - 2.49E+05
      - 4.75E+05

- $t=0.0515s$
  - **STRESS 3**
    - Min = $-2.07 \times 10^6$
    - Max = $9.43 \times 10^5$
    - Color Scale:
      - -1.64E+06
      - -1.21E+06
      - -7.77E+05
      - -3.47E+05
      - 8.33E+04
      - 5.13E+05
Two remarks on conserving scheme:

- same formal order of accuracy as Mid-Point rule
- “conserving” modification cures coupling/stability problem
GENERAL CONSERVING SCHEMES

\[ \dot{z} = J(z) \nabla H(z) - D(z) \nabla H(z) \]

\[ z \in \mathbb{R}^m, \quad H : \mathbb{R}^m \to \mathbb{R}, \]

\[ J = -J^T \in \mathbb{R}^{m \times m}, \quad D = D^T \geq 0 \in \mathbb{R}^{m \times m} \]

• Abstract framework based on “discrete gradients”
• can treat arbitrary integrals
• carries over to infinite-dimensions
Discrete Gradients

Definition

\[ dH : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^m \] is a discrete gradient of \( H \) if

1) \( dH(x, y) \cdot (y - x) = H(y) - H(x), \quad \forall x, y \in \mathbb{R}^m \)

2) \( dH(x, x) = \nabla H(x), \quad \forall x \in \mathbb{R}^m \)

Example

\[
dH(x, y) = \nabla H(\frac{x + y}{2}) + \left[ \frac{H(y) - H(x) - \nabla H(\frac{x+y}{2}) \cdot (y - x)}{|y - x|^2} \right] (y - x)
\]
General Conserving Scheme

To approximate

\[
\dot{z} = J(z) \nabla H(z) - D(z) \nabla H(z)
\]

consider

\[
\frac{z_{n+1} - z_n}{\Delta t} = J(z_{n+\frac{1}{2}}) dH(z_n, z_{n+1}) - D(z_{n+\frac{1}{2}}) dH(z_n, z_{n+1})
\]

where \( z_{n+\frac{1}{2}} = \frac{1}{2}(z_{n+1} + z_n) \).

**Key Features**

Energy decay/conservation

\[
\frac{H(z_{n+1}) - H(z_n)}{\Delta t} = \frac{dH(z_n, z_{n+1}) \cdot (z_{n+1} - z_n)}{\Delta t}
\]

\[
\quad = dH \cdot [JdH - DdH]
\]

\[
\quad = -dH \cdot DdH \leq 0
\]

and

\[
\frac{H(z_{n+1}) - H(z_n)}{\Delta t} = 0 \quad \text{when} \quad D \equiv O.
\]
Momentum conservation (linear/angular momentum)

Suppose

- \( H = \hat{H} \circ \zeta \)
- \( \zeta : \mathbb{R}^m \to \mathbb{R}^k \) invariants under a symmetry group, e.g.
  \[ \zeta(z) = (|q|^2, q \cdot p, |p|^2), \quad z = (q, p) \in \mathbb{R}^6 \]
  "rotational invariants"

- \( F(z) \) an integral associated with \( \zeta \), i.e. \( J \nabla F \in \text{ker}[\nabla \zeta] \)

Result

\[
\begin{array}{|c|c|}
\hline
\zeta(z), F(z) \text{ at most quadratic} & \oplus \\
\hline
\end{array}
\]

“composed” discrete gradient \( d^e H = d\hat{H} \circ \nabla \zeta \)

\[ \downarrow \]

conservation of \( F, H \) when \( D \equiv O \)

Two remarks:

- internal force \( d\hat{H}(\zeta_n, \zeta_{n+1}) \) depends only on invariants
- order of accuracy same as Mid-Point rule
Closing Remarks

• Why does the Mid-Point Rule fail?
  ⇒ artificial coupling between internal forces/rotations

• Is there a cure?
  ⇒ decoupled discretization ⊕ discrete gradients

• Why preserve decay inequalities and integrals?
  ⇒ enhanced stability
  ⇒ useful for constrained systems:

  \[
  \begin{array}{c|c}
  \text{Lagrangian} & \text{Hamiltonian} \\
  \oplus & \oplus \\
  \text{config constraints} & \text{integrals}
  \end{array}
  \]

• Other application for discrete gradients:
  ⇒ discrete gradient flow

  \[
  \frac{z_{n+1} - z_n}{\Delta t} = -dF(z_{n+1}, z_n)
  \]

  "generates strictly decreasing sequence"

  \[
  F_{n+1} - F_n = -\Delta t \left| dF \right|^2 < 0
  \]

  \[
  dF = 0 \iff \nabla F = 0
  \]